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UNITED STATES GOVERNMENT

Memorandum

TO



STATINTL

DATE: Aug. 31, 1972

FROM

: Yale

SUBJECT: Working Group on Chemical Catalysis

Attached is another proposal from the US side. FYI, the initials "PJL" at the end are for Peter J. Lucchesi, Director of Corporate Research for Esso Research and Engineering.

Since there is no chance of getting your opinion before the Joint Working Group ends its meeting tomorrow, you can get the opinion back to me next week some time. I do not believe the Joint Working Group will reach any final decisions at its current meeting, and a second meeting will probably be necessary.

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PROPOSAL "TV"

A Systems Approach to Chemical Catalysis

1. Statement of Proposed Project: Many diverse chemical and instrumental techniques, as well as concepts drawn from metalorganic chemistry, physics, etc., have been applied by different workers to chemical catalysis. However, limitation of resources, standardization methods, etc., have made a truly coordinated or "systems" study difficult, if not impossible. The present exchange program offers an opportunity for such a unified approach by the sharing of resources and skills.

It is proposed to carry out such a coordinated study in order to develop unifying concepts in chemical catalysis. The approach involves choosing a small number of well-studied reactions and probing their detailed catalysis by many of the modern tools and disciplines now being applied by different workers in different locations.

2. Objectives of the Project. This has been described above.
3. Description of Activity: The reactions to be studied would be chosen from (preferably) two of the following:
 - Oxidation of simple (C_2-C_4) olefins
 - Simple acid catalyzed skeletal isomerization of a hydrocarbon
 - Hydrogenation-dehydrogenation of simple hydrocarbon
 - Competitive dehydration-dehydrogenation of alcohols

The choice would be made on the basis of which set of reactions

- provide the greatest generality from the point of view of advancing the field,
- have been most studied and are best understood in homogeneous as well as heterogeneous catalysis.

Once the reactions are chosen, it will be productive to choose the methods most suited to elucidate the mechanism, including:

- Spectroscopic methods
- Comparison of kinetic parameters and mechanisms between solution (metalorganic, acid-base, etc.) and surface mechanisms
- Chemical characterization of surfaces--i.e., diagnostic reactions
- Tracer studies
- Techniques useful for porous solids--sorption, pore size distribution, phase changes, particle size effects, etc.
- Selective poisoning

Solids and complexes used for the project would be standardized.

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Such a program has never been attempted. It is possible within the scope of this program to envision the whole spectrum of possible mechanisms for cooperation--starting with standardization of samples and techniques, exchange of people, joint development of techniques, and assignment of tasks to each side. The Soviets have been very active in some fields that would be relevant--study of oxides, tracer techniques, kinetics, oxidation reactions, metalorganic catalysts, etc. They could complement the skills and background of U.S. workers nicely.

Initially, we would exchange people and set up standardization procedures. The strategy would be developed jointly. Tasks would be assigned to centers of excellence on both sides and periodic joint discussion of results would be essential. The program is an ambitious one. It is probably best to start with a three-year objective and approach the task via a series of "three-year plans".

Many workers and labs on both sides would be aptly suited. For the Soviets, Boreskov could be the coordinator. On the U.S. side, industrial labs who are willing and have an active basic program in catalysis should participate. Specific names have been suggested by the working group in the proposals already submitted. In any case, it might be better to leave that choice to a joint U.S.-Soviet planning group, which would have the task of working out the detailed program jointly.

4. Previous Contacts Between U.S.-USSR: Only on a scientist-to-scientist basis and by the normal exchange of information that occurs between scientists. Both in the case of metal and non-metal catalysis, and in solution coordination chemistry, the Soviet effort has been active. The Soviets have also been active in certain "characterization" areas--notably sorption, ESR, isotope exchange, etc.
5. Time Frame: This is an ambitious program which could last 10 years and should be approached in stages, via a series of three-year plans. A joint working group should be set up to work out the first phase, a planning activity which should take about 6 months.
6. Cost: The total cost for the U.S. could be 1.5 million dollars, about one-third being spent for the first three-year period. Note this is not out of line with costs estimated for other proposals, since the present proposal actually covers two or three of the others.

PJL/ejp
8/28/72